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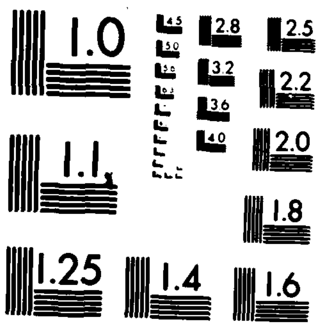

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This is the Final Scientific Report for Air Force Grant AFOSR-81-0193 entitled An Investigation of the Use of Iterative Linear Equation Solvers in Codes for Large Stiff Systems of ODEs. In this report, we highlight the main results we have obtained under the support of this grant. We would like to mention that the continuation of this research is currently being funded by Air Force Grant AFOSR-83-0097. However, this final report will only include results completed under AFOSR-81-193.

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AFOSR-TR- 83-0746 [1]

Final Scientific Report

for Grant AFOSR-81-0193

An Investigation of the Use of Iterative Linear Equation Solvers in Codes for Large Stiff Systems of ODEs

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Tony F. Chan[1]

July 18, 1983

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Abstract

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Table of Contents

1. Introduction

This project deals with the problem of solving large systems of stiff ODEs. In particular, ~~we see~~ as one of the major issues, the choice of methods for solving the systems of linear and nonlinear equations that arise at each integration step. ~~We~~ proposed to use variants of the preconditioned conjugate gradient (PCG) method for solving the linear equations, and truncated Newton-like iterations for solving the nonlinear equations. Our main objective is to carry out a systematic study of the methods involved and ultimately to produce a well-documented and well-tested computer code for solving large systems of stiff ODEs that incorporates the results of our study. A brief summary of our original proposed research will be given in Section 2.

In the 17 months (1 year plus 5 months no-cost extension) supported by this grant, we believe we have made definite progress towards our ultimate goal. We have developed some fundamental algorithms in the area and produced a first version of the program package that incorporates PCGPACK with LSODE. Highlights of the results accomplished will be presented in Section 3. A total of five technical reports have been produced under this grant, of which three ~~have been~~ accepted for publications in SIAM journals, and one is near completion. Copies of these reports have already been submitted to AFOSR before and will not be included with this final report.

2. Goals of the Project

~~Our~~ main objective is to determine whether the use of *iterative* methods for solving linear systems of algebraic equations in codes for large stiff systems of ODEs is competitive with sparse *direct* techniques. A more tangible objective is to produce a computer program that incorporates such an approach. There are at least four main issues that have to be investigated:

1. Which preconditioned conjugate gradient method is the best for our purpose? (Which variants of the method: Conjugate Gradient or Conjugate Residual? Which of the many nonsymmetric variants? Which preconditionings?)

2. What is the best way to solve the nonlinear systems? (Newton-like methods, truncated versions, chord versions, directional differencing, efficient evaluation of the Jacobian.)

3. How to modify the formula, strategies, and heuristics of the ODE solver to take advantage of the greater freedom offered by the iterative methods? (Variable coefficient formulas, more frequent change of step size and order.)

4. How does a code based on our approach compare with the existing codes in its performance on real problems? (Electrical network problems, Method of Lines for PDEs.)

3. Highlights of Results

3.1. Alternating Direction Incomplete Factorizations

The use of a good preconditioning is often essential for the successful application of the conjugate gradient method. One of the most promising class of preconditionings is the so-called **Incomplete Factorizations,** which can be viewed as factoring the coefficient matrix approximately under the constraint that the factors have to be sparse. For elliptic PDEs, quite a lot of theory has been developed for these preconditionings. Most of these preconditionings have the property that, when applied to the discretization of a self-adjoint elliptic opertor, the number of iterations required to reduce some norm of the error by a factor of ϵ is $O(h^{-1/2}\log(1/\epsilon))$, where h is the mesh size used in the discretization. By modifying one of these preconditionings, namely, the Dupont-Kendall-Rachford preconditioning (DKR), we have been able to derive some error estimates which suggest that the number of iterations can be reduced to $O(h^{-1/3}\log(1/\epsilon))$. Thus this new preconditioning, which we call ADDKR, is *asymptotically* faster than DKR. Moreover, numerical experiments on some model elliptic problems indicate that even for problems of moderate size the new preconditioning is competitive with DKR. We feel that this is an important discovery, both theoretically and practically, *since no other known preconditionings in this class have been shown to possess a better asymptotic rate of convergence than DKR.* This work appeared in the SIAM Journal of Numerical Analysis in April, 1983.

3.2. Nonlinear Preconditionings

One promising idea that some people have noticed in the application of Krylov subspace methods for solving the linear systems $Aw = b$ that arise in the inner loop of a Newton-like iterative method for solving nonlinear systems $F(x) = 0$ (with A being the Jacobian of F at a point x) is the use of the **directional differencing** $(F(x + \epsilon u) - F(x)) / \epsilon$ for approximating the matrix-vector product Au in the CG algorithm. This avoids explicit evaluations of the Jacobian and only requires function evaluations. However, most of the preconditioning techniques in use now are derived from the matrix elements *explicitly*. It is therefore unclear as to how to apply the preconditionings when the matrix is not explicitly available. This issue does not seem to have been addressed in the literature. We have obtained some results in this direction. We have derived an algorithm for preconditioning the CG iteration with directional differencings that reduces to the SSOR preconditioning in the linear case. It only requires evaluating the diagonal elements of the Jacobian which can also be approximated by function evaluations and can be easily incorporated into the CG iteration. We consider it an important discovery because we think the use of directional differencing will prove to be very useful in the stiff ODE context. We plan to incorporate the results into the final version of our code. We presented a talk on this topic

in the Sparse Matrix Symposium held in Fairfield Glade, Tennessee in October, 1982. The paper has been accepted for publication in the SIAM Journal of Scientific and Statistical Computing.

3.3. Basic CG Variant of LSODE

All versions of our code are going to be built around and incorporated into the package LSODE by Alan Hindmarsh. A first version of the code has been completed. It basically replaces the sparse matrix solver in LSODE with the conjugate gradient solver PCGPACK developed at Yale. The code, with we call LSODECG, can now take problems in the sparse format (same as the IA-JA format used in the Yale Sparse Matrix Package (YSMP) and in LSODES) and solves the linear systems that arise at each integration step by variants of the preconditioned conjugate gradient method. It computes the Jacobian exactly by rows and uses absolute error control. One of the more subtle issues is the control of the various levels of iterations in the code: the ODE step, the nonlinear iteration at each step and the linear CG iteration at each nonlinear iteration. For example, the stopping criterion for the conjugate gradient method has to be related to the user supplied error tolerance for the ODEs. We have obtained some very useful results in this direction.

Another unexpected discovery is that in solving the linear system $(I - h\beta J)x = b$ at each integration step, where x is the change in the Newton iterates, it seems to be better to take as initial guess for x the right hand side b rather than the natural choice of the zero vector. An intuitive explanation for this is that the coefficient matrix is approximately equal to the identity matrix in the subspace of the small eigenvalues of J whereas the component of x in the dominant subspace is small outside the transient regions. Therefore, the right hand side b is a good approximation to the solution x. This has very important practical implications since it appears to reduce the number of CG iterations greatly.

We have performed some preliminary tests on LSODECG with problems in the STIFF DETEST program (developed at the University of Toronto for testing stiff ODE solvers) and on some model PDEs. Our main objective is to compare it the sparse option LSODES in the LSODE package. These preliminary results seem to confirm the effectiveness of the use of CG-like methods, especially for larger problems like those arising from 3-D PDEs. For simple 2-D PDEs, however, it seems difficult to beat LSODES. This is because, for smooth problems where LSODES can get away with frequently not refactoring the Jacobian matrix and reusing an old factorization in a chord Newton iteration, the factorization cost becomes negligible and this makes LSODES very efficient on such problems. We expect the situation will be more in LSODECG's favor for more difficult problems where the Jacobian matrix changes more frequently.

A report on these results is under preparation and should be available towards the end of summer, 1983.

3.4. Lanczos Method for Multiple Right Hand Sides

In the stiff ODE context, it is important to be able to deal with systems with multiple right hand sides. This is because the right hand sides are usually not available simultianeously as they depend on the solution of the previous system. One way of achieving improved efficiency is by saving the Krylov subspaces generated for the previous systems and reusing them in subsequent solutions, as proposed by Parlett. We have obtained some results in this direction. We showed that one of the algorithms proposed by Parlett is theoretically equivalent to the Block Lanczos method. A technical report on this topic has been completed.

3.5. Comparison of Krylov subspace methods

A host of algorithms belonging to the same class of Krylov subspace methods have been recently at the focus of several researchers dealing with the solution of large sparse unsymmetric systems. Among them we mention the subclass of the ORTHOMIN(k)(Vinsome), GCR(k) algorithms, (Eisenstat, Elman and Schultz). ORTHORES(k), ORTHODIR(k) developed by Young and Jea, IOM(k) (Saad), Axelsson's method, Lanczos' method and others. Although the literature is rich in methods, few comparisons of the performances have been proposed. In the particular context of stiff ODE the choice of a method is even less clear.

In a recent paper, we have performed some comparisons with a class of Krylov subspace methods, both theoretically and empirically. In particular, it was shown that the ORTHORES(k) method of Jea and Young is in fact equivalent to the IOM(k) method, i.e. the iterates produced by both algorithms are identical. On the other hand both numerical stability and computational cost are in favor of the IOM(k) algorithms. A number of comparisons shown in Howard Elman's recent PhD thesis at Yale favor the Chebychev based algorithms, in general, against the Conjugate Gradient type methods. A common argument raised against the Chebychev algorithm is that it requires the knowledge of some of the eigenvalues of A. While there is no doubt that the process of estimating the eigenvalues and obtaining the best ellipse containing the spectrum of A may seem somewhat cumbersome, there are a few important points that can make the process highly competitive:

1. Once the optimal parameters are known, the method is extremely fast,
2. Hybrid methods combining conjugate gradient type method to estimate eigenvalues together with subsequent use of Chebychev type methods may turn out to be very efficient,
3. In the stiff ODE context, the problem of estimating the parameters is eased by the fact that they are likely to evolve smoothly thus allowing the use of a set of parameters for a large number of integration steps.

Although the choice of the best iterative method in the stiff ODE context is still far from resolved, and it may

never be, we feel that we have a much better understanding of the relative performance of the various algorithms now. The paper describing this work has been accepted to appear in the SIAM Journal of Sci. Stat. Comp.

4. List of reports supported by AFOSR-81-0193

1. "Alternating Direction Incomplete Factorizations" by Tony F. Chan, Ken Jackson and Benren Zhu, SIAM J. Numer. Anal., Vol.20, No.2, April, 1983.
2. "Nonlinearly Preconditioned Krylov Subspace Methods for Discrete-Newton Algorithms" by Tony F. Chan and Ken Jackson, accepted to appear in SIAM J. Sci. Stat. Comp.
3. "On the Lanczos Algorithm for Solving Symmetric Linear Systems with Several Right Hand Sides" by Youcef Saad, Yale Computer Science Technical Report.
4. "Practical Use of Some Krylov Subspace Methods for Solving Indefinite and Unsymmetric Linear Systems" by Youcef Saad, accepted to appear SIAM J. Sci. Stat. Comp.
5. "The Numerical Solution of Large Systems of Stiff ODEs" by Tony F. Chan and Ken Jackson, paper presented at SIAM National meeting at Stanford in July, 1982. Technical report under preparation.

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